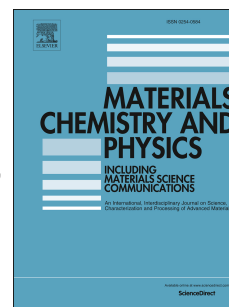


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Database development and Calphad calculations for high entropy alloys: challenges, strategies, and tips

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Abstract

The development of a reliable multicomponent thermodynamic database for high entropy alloys (HEAs) is a daunting task and it faces new challenges comparing to the development of databases for conventional single principal element alloys, such as the assessment of a large number of ternary systems, the proper estimation of phase stability within metastable compositional and temperature ranges, and the reasonable extrapolation into higher order systems. We have recently established a thermodynamic database (TCHEA1) especially for HEAs within a 15-element framework. This work highlights the usage of high throughput density functional theory (DFT) calculations for validating and refining the binary and ternary parameters of the solid solution phases, and having a more reliable extrapolation into metastable regions and higher order systems. TCHEA1 consists of 105 binaries and 200 ternaries and contains nearly all the stable solution phases and intermetallic compounds in each of the assessed systems. Together with Thermo-Calc, this database enables us to predict the stability of the desired multicomponent solid solution relative to intermetallic compounds and other solid solutions. Calculation examples are presented not only for case studies but also for bridging the knowledge gap between Calphadian and people who do not have a background of the Calphad approach.

Keywords: High entropy alloys; Calphad; thermodynamic database; thermodynamic calculation

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